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Published in:
Journal of Applied Physics

DOI:
10.1063/1.1555269

Publication date:
2003

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Citation: Journal of Applied Physics **93**, 3668 (2003); doi: 10.1063/1.1555269
View online: https://doi.org/10.1063/1.1555269
View Table of Contents: http://aip.scitation.org/toc/jap/93/6
Published by the American Institute of Physics

On erbium lattice location in ion implanted $Si_{0.75}Ge_{0.25}$ alloy: Computer simulation of Rutherford backscattering/channeling

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(Received 22 May 2002; accepted 3 January 2003)

A high crystalline quality $Si_{0.75}Ge_{0.25}$ alloy layer grown by chemical vapor deposition was implanted with 70 keV Er^+ ions to a fluence of $10^{15}\,cm^{-2}$ at temperature of 550 °C. The implantation was found to result in an Er depth distribution with 1 at. % maximum concentration 30 nm beneath the surface. The location of the erbium atoms in the host matrix lattice is derived through computer simulation of experimental axial channeling angular scans measured by *in situ* Rutherford backscattering/channeling spectrometry. Using computer code FLUX 7.7 it is shown that 60% of the implanted erbium atoms are located at ytterbium sites, 10% at tetrahedral sites, and the remainder are associated with random locations in the host matrix. © *2003 American Institute of Physics.*
[DOI: 10.1063/1.1555269]

At present, there is an urgent need for high efficiency optical emitters that are compatible with conventional ultralarge scale integration (ULSI) silicon based technology. Since silicon is known to have an indirect gap, it is a fundamentally inefficient light emitter compared with direct gap semiconductors such as gallium arsenide and other III–V compounds. However, it is much more expensive to fabricate devices using III–V semiconductors because different processing techniques are needed and these are not compatible in general with mature, highly developed contemporary silicon based technology. Silicon devices completely dominate the microelectronics market because of their low manufacturing cost.

Over the past decade a great deal of attention has been given to the study of how silicon can be modified to allow the use of alternative silicon based schemes for optoelectronics. There is some hope that quantized systems (superlattices and heterostructures, silicon nanosized precipitates and quantum dots, porous silicon, and irradiation induced charge carrier spatial confinement) and schemes based on rare-earth elements doping, e.g. of erbium, will offer a way by which to develop efficient silicon based light emitters both in the visible and infrared regions. Recently, optical properties of Er doped semiconductors have attracted a lot of attention due to their potential application for the fabrication of advanced optoelectronic devices. Virtually independent of the host matrix, incorporated erbium in its trivalent state Er^{3+} emits light at a wavelength of 1.54 μm due to a $^4I_{13/2}-^4I_{15/2}$ electronic transition. Since the line corresponds to the minimum of optical absorption of silica, a material used for optoelectronic interconnections and in optocommunications, Er is of particular interest for the doping of silicon based structures. However, at present two major factors prevent Si:Er devices produced so far from reaching light emission that is efficient enough for application. First, $^4I_{13/2}-^4I_{15/2}$ electronic transition is forbidden for an insolated Er atom and becomes possible only due to a crystal lattice field. Consequently, the long radiative lifetime results in a moderate luminescence yield. Second, erbium is characterized by very low solubility in silicon based material and, therefore, the maximum concentration of optically active Er atoms attainable by conventional methods such as doping during molecular beam epitaxial growth is limited by equilibrium thermodynamical phase diagrams. In contrast to Si, in a $Si_{1-x}Ge_x$ host the emission can be optimized by varying the band gap energy as a function of the Ge concentration and thus energy transfer can reach acceptable levels. By adding only few percent of germanium, $Si_{1-x}Ge_x$ allows one to manipulate the electronic and optical properties. Therefore, $Si_{1-x}Ge_x$ alloys constitute a promising material for the fabrication of next generation optoelectronic devices with high compatibility with conventional ULSI silicon technology. Since ion implantation by nature is a nonequilibrium process, it can be used to extend the concentration of optically active Er atoms in $Si_{1-x}Ge_x$ alloys well beyond the terminal equilibrium solid solubility limit. In spite of the fact that data on both photoluminescence and electroluminescence from Er doped Si, Si–Ge, SiO_2, and Si/Si–Ge based heterostructures are available in the literature, it is still not well known what the lattice location of optically active Er atoms actually is in various host matrices.

In a previous letter we reported an experimental study of the Er lattice location in an ion implanted $Si_{0.75}Ge_{0.25}$ alloy using Rutherford backscattering (RBS)/channeling spectrometry. A high-quality crystalline $Si_{0.75}Ge_{0.25}$ layer with a (100) surface and thickness of around 1 μm was grown by chemical vapor deposition on top of a compositionally graded $Si_{1-x}Ge_x$ buffer with x ranging from 0 to 0.25. The buffer resided on a *p*-type Si(100) substrate with resistivity of less than 0.02 Ω cm. The high quality of the crystal layer structure grown was ensured by RBS/channeling prior to implantation. The alloy was implanted with 70 keV Er^+ ions in a random direction to a fluence of $10^{15}\,cm^{-2}$. Implantation was performed at temperature of 550 °C in order to avoid

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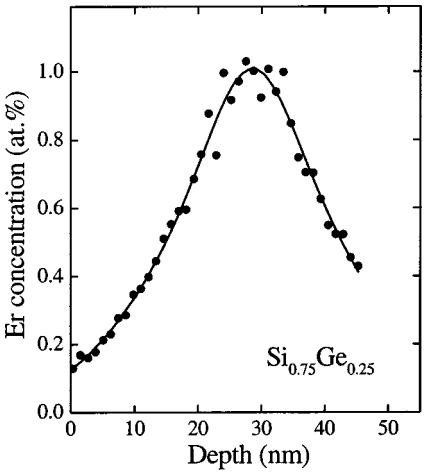

FIG. 1. Erbium depth profile in a $Si_{0.75}Ge_{0.25}$ alloy after implantation of 70 keV Er^+ ions at 550 °C to a fluence 10^{15} cm^{-2}. The line is to guide the eye.

irradiation induced amorphization which is otherwise unavoidable at such high fluence. RBS/channeling measurements using a 500 keV He^{2+} beam were carried out *in situ* at room temperature (RT) to analyze the channeling characteristics of the implanted layer.

The implantation is seen in Fig. 1 to result in a depth distribution of Er atoms with maximum concentration close to 1 at. % at a depth of 30 nm. The depth profile was calculated by simulating a corresponding experimental RBS spectrum. Integration of the Er content over the distribution assured the retention of an Er fraction close to 100% for the fluence used. He^{2+} ions channeling in the implanted layer between 10 and 40 nm is shown in Fig. 2. Axial channeling angular scans for ⟨100⟩, ⟨110⟩, and ⟨111⟩ directions, i.e., RBS yields normalized to randomly backscattered spectra as functions of the tilt angle around the corresponding crystallographic axes, are presented in the figure for Er, Si, and Ge. The low values of the minimum normalized RBS yields for Si and Ge, i.e., for He^{2+} ions incident along the low index crystallographic axis, indicate that keeping the sample at 550°C during implanting essentially prevented irradiation induced amorphization by high temperature stimulated spontaneous recovery of the matrix crystallinity. The angular scans for Er revealed 20% channeling in the ⟨100⟩ direction and 9% in the ⟨111⟩. In contrast, the ⟨110⟩ axis is characterized by strong backscattered flux that is seen to peak in the middle of the channel with adjacent shoulders.

In our previous study[1] the peculiarities observed in the angular scans for Er were ascribed to Er atoms at tetrahedral interstitial lattice sites. However, unambiguous identification of the location of an impurity in a crystal directly from ion channeling angular scans is possible only in trivial cases for lattice sites with high symmetry. Further investigation has revealed that the case of Er in silicon germanium turns out to be much more complicated and this might be the reason for the disagreement in the literature on specific lattice sites Er atoms can occupy in silicon based matrices. Although emission channeling experiments showed evidence of the theoretically predicted[2] tetrahedral interstitial location[3] in silicon, ion channeling, on the other hand, detected Er atoms only on substitutional and hexagonal interstitial sites.[4,5]

In order to identify more accurately the lattice location of Er implanted into a $Si_{0.75}Ge_{0.25}$ alloy, we have performed computer simulation of the axial channeling angular scans with the FLUX code. A detailed description of the basic version of the code is presented elsewhere.[6] The code was modified and adapted to a silicon germanium host matrix. In an upgraded version, FLUX 7.7, an option was added that allows mixed lattices such as $Si_{1-x}Ge_x$. This option also enables one to introduce vacancies into the lattice. Another improvement is an update of the cross section option adapted to handle layered crystals, as well as mixed lattices, with different cross sections for each atom species.

The simulation parameters were set to correspond to the experimental conditions and 90 000 ions were followed in calculations for each selected channeling direction. For He ions with energies from 500 to 300 keV used in the calculations the Rutherford cross section was assumed to be accurate enough. Although implantation at 550 °C in our experiments prevented amorphization of the $Si_{0.75}Ge_{0.25}$ sample, its crystallinity, however, was impaired by high fluence irradiation. We assume that most of the residual damage in the sample was due to irradiation generated point defects, since no extended defects were observed in the as-implanted sample by electron transmission microscopy. Irradiation induced damage was taken into account in the simulation by introducing randomly distributed vacancies and layered structures of various vacancy complexes into the host lattice

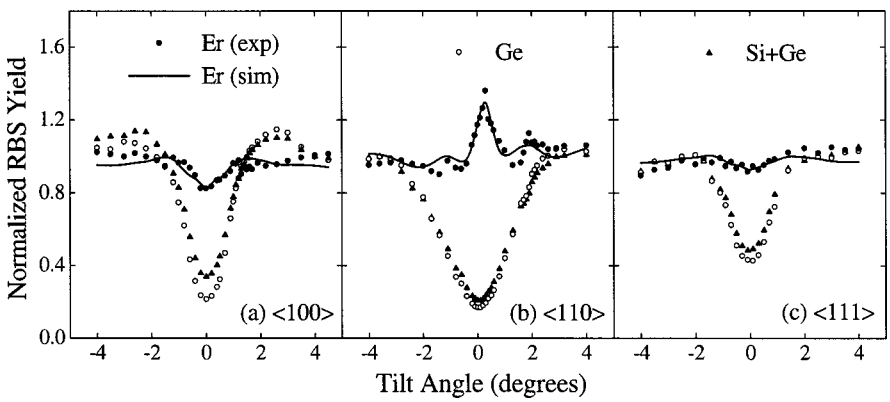

FIG. 2. Axial channeling angular RBS scans around (a) ⟨100⟩, (b) ⟨110⟩, and (c) ⟨111⟩ crystallographic axes for Er, Si, and Ge.

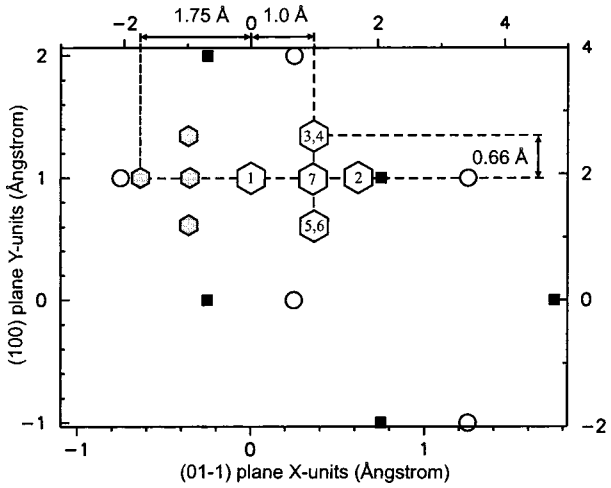

FIG. 3. Schematic projection of a silicon germanium diamond crystal lattice on the plane perpendicular to the ⟨110⟩ direction. ○ and ■ denote either Si or Ge atoms, respectively, of the host lattice that correspond to different layers. Two sets of Er atoms at tetrahedral (7) and ytterbium (1, 2–6) sites that correspond to different layers are shown by open and shaded hexagons, respectively.

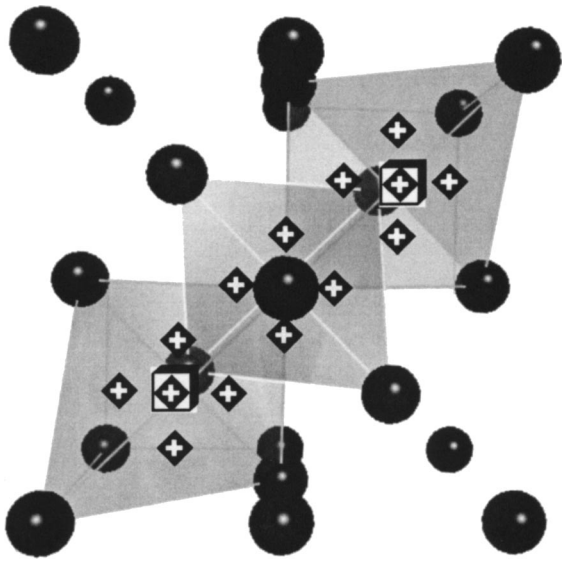

FIG. 4. Isometric presentation of a silicon germanium lattice with Si and Ge atoms denoted by closed circles. Crosses and cubes confined within tetrahedrons show interstitial ytterbium and tetrahedral sites, respectively, where Er atoms were found to be located in a $Si_{0.75}Ge_{0.25}$ host matrix.

and by using vibrational amplitudes of the matrix atoms and beam divergence as fitting parameters.

Simulated angular scans are presented for Er in Fig. 2 by solid lines. The correspondence between experimental and calculated scans is seen to be rather good. In order to fit the experimental data, $10\pm5\%$ of the Er atoms had to be located at tetrahedral interstitial sites [T sites with coordinates $(1/2, 0, 0)$, $(1/2, 1/2, 1/2)$, and $(1/4, 1/4, 3/4)$ in a quarter unit cell in the Si–Ge lattice], $60\pm8\%$ at ytterbium interstitial sites [Y sites: $(T)\pm(1/8, 0, 0)$], and the remainder distributed randomly in the matrix. Although the calculations were extremely sensitive to the Er lattice location, positioning of the impurity atoms at ytterbium sites was tolerated within an uncertainty of ±0.1 and ±0.25 Å for tetrahedral sites. In Fig. 3, for example, the configuration of Er sites that fits the experimental data the best is presented. Figure 3 shows the (110) projection of the silicon germanium lattice with Si and Ge atoms corresponding to different layers, depicted by squares and circles, respectively. Open hexagons denote Er atoms at slightly shifted tetrahedral (7) and ytterbium sites (1, 2–6). Closed hexagons show the same configuration corresponding to different layers. An isometric view of the Er sites layout is shown in Fig. 4. The potential lattice sites, that Er atoms can occupy in silicon germanium matrix, are seen to concentrate around regular interstitial tetrahedral sites. This is not unexpected since oversized Er atoms implanted into a rigid silicon germanium lattice introduce stress that is reduced by energetically favorable accommodation of the impurity at tetrahedral and ytterbium sites.

The potential Er lattice sites revealed in this work might be of importance for developing methods to inhibit so-called concentration quenching of light emission observed in Er doped silicon based structures used in optoelectronics, e.g., for optical amplifiers, on-chip interconnections, fibers, etc. In order to increase the emission efficiency, the concentration of optically active Er atoms should be sufficiently high. However, due to the limited solid solubility of Er in silicon based material, doping with high concentrations may lead to the clustering of Er atoms and the subsequent formation of nanosized precipitates. Er atoms confined within the precipitates are no longer optically active because of interactions between closely spaced Er atoms, which leads to nonradiative electron transitions. Consequently, concentration quenching can significantly degrade the light emission efficiency by reducing the amount of optically active Er. Since Er atoms were found to be located at tetrahedral and ytterbium sites in a diamond cubic crystalline matrix, one may speculate that simultaneous codoping with another element that tends to occupy the same type of lattice location, e.g. Yb, might effectively reduce the probability for Er atoms to be in close proximity to each other. This might preclude Er from precipitation and allow one to extend the Er solid solubility beyond the thermodynamical equilibrium limit towards a supersaturated solution, thereby minimizing the detrimental effect of concentration quenching on the light emission efficiency.

In summary, we have used the RBS/channeling technique complemented by computer simulation to study the lattice location of Er implanted into a $Si_{0.75}Ge_{0.25}$ alloy. It was shown that implantation at high temperature can lead to the incorporation of Er atoms at regular interstitial sites in the host matrix. Specific lattice positions that Er can occupy were identified and they were found to be concentrated around interstitial tetrahedral sites in the host matrix.

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